

2-Butenal, 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-

Other names:

Boronia butenal

2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-butenal

Inchi: InChI=1S/C14H22O/c1-11(10-15)7-8-13-12(2)6-5-9-14(13,3)4/h7,10H,5-6,8-9H2,1-4H3/b

InchiKey: FJCQUJKUMKZEMH-YRNVUSSQSA-N

Formula: C14H22O

SMILES: CC(C=O)=CCC1=C(C)CCCC1(C)C

Mol. weight [g/mol]: 206.32

CAS: 3155-71-3

Physical Properties

Property code	Value	Unit	Source
gf	68.81	kJ/mol	Joback Method
hf	-206.04	kJ/mol	Joback Method
hfus	19.18	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.048		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpola	1584.20		NIST Webbook
rinpola	1584.00		NIST Webbook
rinpola	1584.20		NIST Webbook
tb	601.33	K	Joback Method
tc	815.54	K	Joback Method
tf	327.58	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.74	J/molxK	601.33	Joback Method
cpg	506.02	J/molxK	637.03	Joback Method
cpg	523.29	J/molxK	672.73	Joback Method
cpg	539.68	J/molxK	708.44	Joback Method

cpg	555.31	J/mol×K	744.14	Joback Method
cpg	570.31	J/mol×K	779.84	Joback Method
cpg	584.81	J/mol×K	815.54	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3155713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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